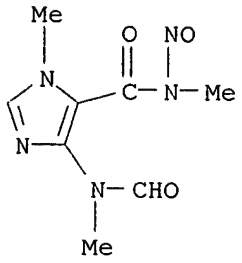
L Number	Hits	Search Text	DB	Time stamp
1	154	(548/326.5).CCLS.	USPAT; US-PGPUB; EPO; JPO	2002/06/03 10:04

V. Balasubramanian



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

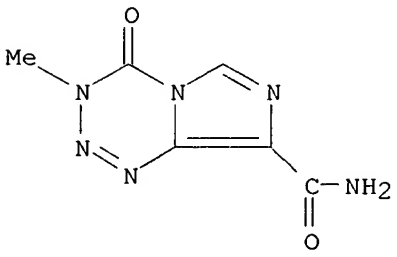
=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.76	0.97

STN INTERNATIONAL LOGOFF AT 12:56:01 ON 03 JUN 2002

V. Balasubramanian

AN 1999:794749 CAPLUS
DN 132:151791
TI Pyrrolo[2,1-d][1,2,3,5]tetrazines, a new class of azolotetrazines related to the antitumor drug temozolomide
AU Diana, Patrizia; Barraja, Paola; Lauria, Antonino; Almerico, Anna Maria; Dattolo, Gaetano; Cirrincione, Girolamo
CS Dipartimento Farmacochimico-Tossicologico Biologico, Univ. Studi Palermo, Palermo, I-90123, Italy
SO Synthesis (1999), (12), 2082-2086
CODEN: SYNTBF; ISSN: 0039-7881
PB Georg Thieme Verlag
DT Journal
LA English
OS CASREACT 132:151791
AB A series of pyrrolo[2,1-d][1,2,3,5]tetrazines, potential antineoplastic agents, was obtained in good yield from the reaction of 2-diazopyrroles with isocyanates at room temp. and in the dark.[5] At. charges at C(4), a good parameter to predict the antineoplastic activity for this type of compds., are very close to that of temozolomide.
IT **85622-93-1P**, Temozolomide
RL: PNU (Preparation, unclassified); **PREP (Preparation)**
(prepn. and at. charge of pyrrolo[2,1-d][1,2,3,5]tetrazines related to temozolomide)
RN 85622-93-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

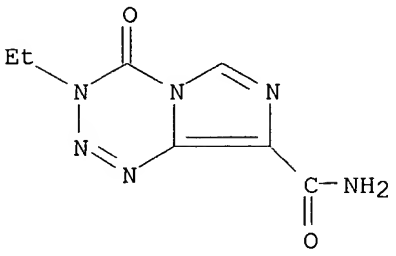
L6 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1998:259743 CAPLUS
DN 129:27924
TI Antitumor imidazotetrazines. Part 36. Conversion of 5-aminoimidazole-4-carboxamide to imidazo[5,1-d][1,2,3,5]tetrazin-4(3H)-ones and imidazo[1,5-a][1,3,5]triazin-4(3H)-ones related in structure to the antitumor agents temozolomide and mitozolomide
AU Wang, Yongfeng; Wheelhouse, Richard T.; Zhao, Linxiang; Langnel, David A. F.; Stevens, Malcolm F. G.
CS School of Pharmaceutical Sciences, Cancer Research Laboratories, Nottingham University, Nottingham, NG7 2RD, UK
SO J. Chem. Soc., Perkin Trans. 1 (1998), (10), 1669-1675
CODEN: JCPRB4; ISSN: 0300-922X
PB Royal Society of Chemistry
DT Journal
LA English

V. Balasubramanian

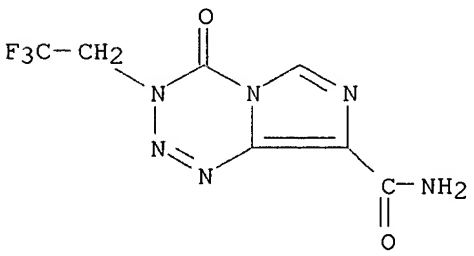
AB Novel 3-substituted imidazo[5,1-d][1,2,3,5]tetrazinones have been prepd. by two routes: reaction of 5-diazoimidazole-4-carboxamide and isocyanates, and nitrosative cyclization of 5-amino-1-carbamoylimidazole-4-carboxamides. The latter cyclizations do not proceed efficiently when the 1-carbamoyl group bears an electron-donating alkyl group. 5-Amino-1-carbamoylimidazole-4-carboxamides cyclize with tri-Et orthoformate or tri-Et orthobenzoate to yield imidazo[1,5-a][1,3,5]triazinones. A 1H NMR study of the decompn. of 8-carbamoyl-3-ethylimidazo[5,1-d][1,2,3,5]tetrazin-4(3H)-one in deuteriated phosphate buffer has shown that its ethylating capacity is attenuated by the unproductive generation of ethene. This observation explains why the ethylimidazotetrazine possesses weaker antitumor properties than the clin.-used congener temozolomide.

IT **97716-74-0P 208107-15-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of imidazo[5,1-d][1,2,3,5]tetrazin-4(3H)-ones and imidazo[1,5-a][1,3,5]triazin-4(3H)-ones)

RN 97716-74-0 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-ethyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

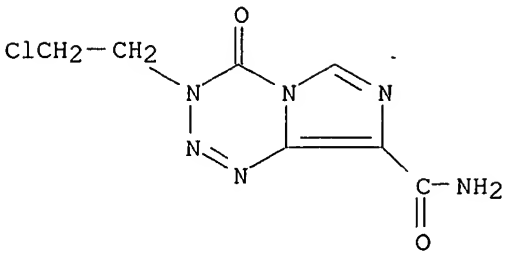


RN 208107-15-7 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

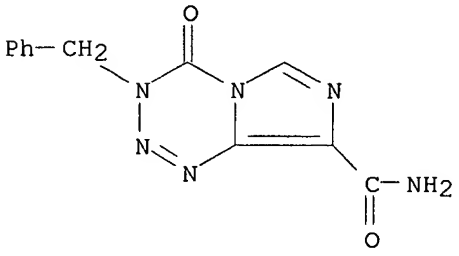


IT **85622-95-3P**, Mitozolomide **85623-02-5P 208107-14-6P 208107-16-8P 208107-17-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of imidazo[5,1-d][1,2,3,5]tetrazin-4(3H)-ones and imidazo[1,5-a][1,3,5]triazin-4(3H)-ones)

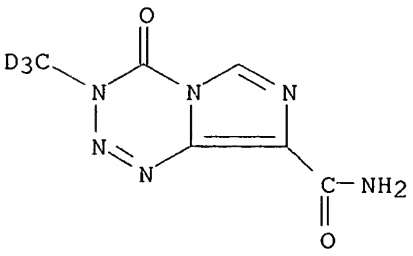
RN 85622-95-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



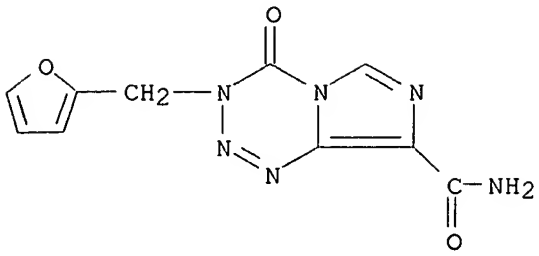
RN 85623-02-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



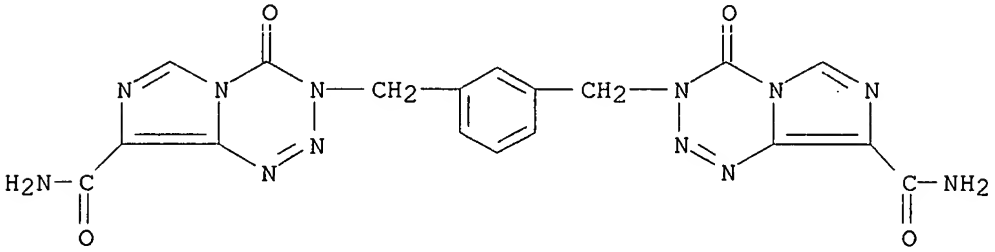
RN 208107-14-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(methyl-d3)-4-oxo- (9CI) (CA INDEX NAME)



RN 208107-16-8 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-furanylmethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

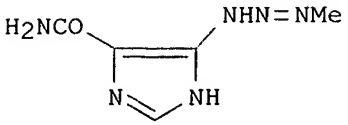


RN 208107-17-9 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,3'-[1,3-phenylenebis(methylene)]bis[3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

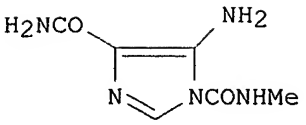


L6 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1997:684618 CAPLUS
DN 127:293195
TI Antitumor Imidazotetrazines. 35. New Synthetic Routes to the Antitumor Drug Temozolomide
AU Wang, Yongfeng; Stevens, Malcolm F. G.; Chan, Tze-ming; DiBenedetto, Donald; Ding, Zhe-xing; Gala, Dinesh; Hou, Donald; Kugelman, Max; Leong, William; Kuo, Shen-chun; Mas, Janet L.; Schumacher, Doris P.; Shutts, Bruce P.; Smith, Lyman; Zhan, Zheng-Yun J.; Thomson, William T.
CS Cancer Research Laboratories Department of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK
SO J. Org. Chem. (1997), 62(21), 7288-7294
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
GI

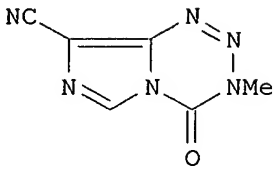
V. Balasubramanian



II



III



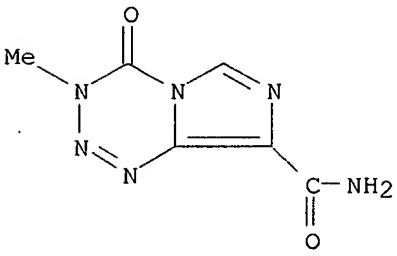
IV

AB Three new pathways to the antitumor drug temozolomide (I) were explored via intermediate imidazolecarboxamides II and III and the imidazotetrazinone IV. The key intermediate III was converted to I in 45% yield by employing NaNO2 in aq. tartaric acid at 0-5.degree.. III was prepd. from 5-amino-1-[[(4-nitrophenyl)oxy]carbonyl]imidazole-4-carboxamide and MeNH2 or directly from 5-aminoimidazole-4-carboxamide and either MeNCO or MeNHCOCl. I was also prepd. from IV by hydrolysis to the HCl salt of I in 10 M HCl. IV was prepd. from either 5-diazoimidazole-4-carbonitrile and MeNCO or by diazotization of 5-amino-1-(N-methylcarbamoyl)imidazole-4-carbonitrile. Attempts to cyclize II with phosgene or phosgene equiv. were unsuccessful and only 2-azahypoxanthine was isolated.

IT **85622-93-1P**, Temozolomide
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of temozolomide by cyclization of imidazolecarboxamides)

RN 85622-93-1 CAPLUS

CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)

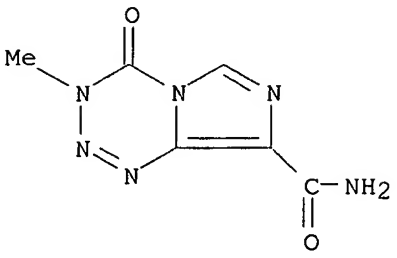


IT **196806-18-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of temozolomide hydrochloride by hydrolysis of cyanotemozolomide)

RN 196806-18-5 CAPLUS

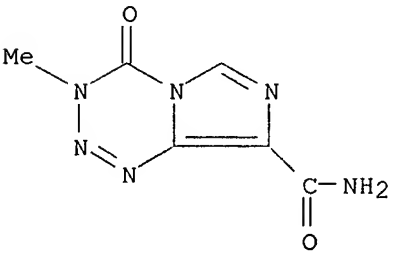
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

V. Balasubramanian



● HCl

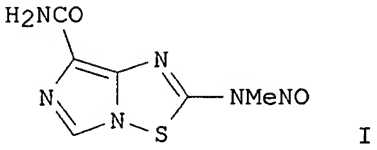
L6 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1997:417852 CAPLUS
DN 127:89996
TI Temozolomide: a review of its discovery, chemical properties, pre-clinical development and clinical trials
AU Newlands, E. S.; Stevens, M. F. G.; Wedge, S. R.; Wheelhouse, R. T.; Brock, C.
CS Dep. Med. Oncology, Charing Cross Hospital, London, W6 8RF, UK
SO Cancer Treat. Rev. (1997), 23(1), 35-61
CODEN: CTREDJ; ISSN: 0305-7372
PB Saunders
DT Journal; General Review
LA English
AB A review with 106 refs. on the synthesis of, mechanism of antitumor activity of and clin. trials with temozolomide.
IT **85622-93-1P**, Temozolomide.
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(temozolomide: discovery, chem. properties, pre-clin. development and clin. trials)
RN 85622-93-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1997:168958 CAPLUS
DN 126:264081
TI A new route to the antitumor drug temozolomide, but not thiotemozolomide

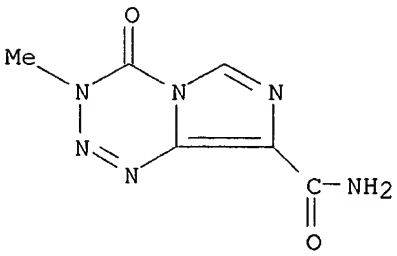
V. Balasubramanian

AU Wang, Yongfeng; Lowe, Philip R.; Thomson, William T.; Clark, Jonathan; Stevens, Malcolm F. G.
CS Cancer Res. Lab., Univ. Nottingham, Nottingham, NG7 2RD, UK
SO Chem. Commun. (Cambridge) (1997), (4), 363-364
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 126:264081
GI

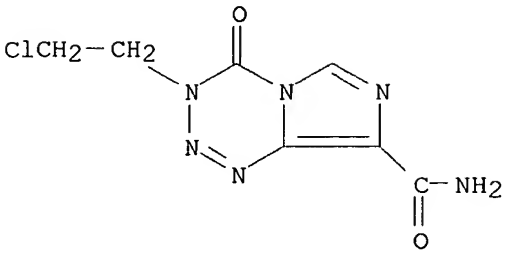


I

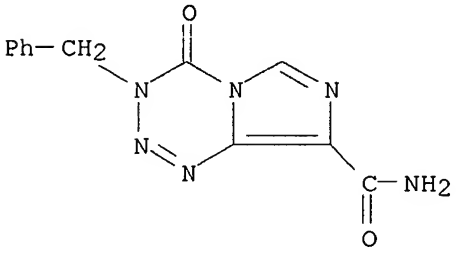
AB Interaction of 5-aminoimidazole-4-carboxamide with alkyl isocyanates yields N-substituted 1-carbamoylimidazoles which can be cyclized to imidazo[5,1-d][1,2,3]tetrazin-4(3H)-ones, including temozolomide, on nitrosation; a similar reaction with Me isothiocyanate, followed by nitrosation, affords the nitrosomethylamino deriv. I of a new ring-system, imidazo[1,5-b][1,2,4]thiadiazole.
IT **85622-93-1P 85622-95-3P 85623-02-5P 97716-74-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of temozolomide and imidazo[1,5-b][1,2,4]thiadiazole deriv.)
RN 85622-93-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



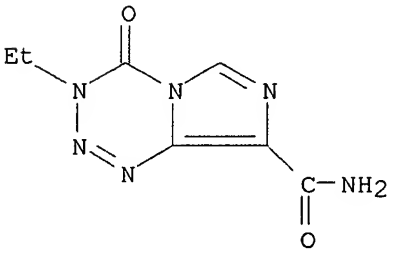
RN 85622-95-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



RN 85623-02-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



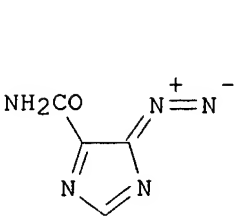
RN 97716-74-0 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-ethyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



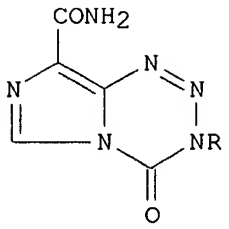
L6 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1996:108643 CAPLUS
DN 124:232405
TI Synthetic studies of 8-carbamoylimidazo-[5,1-D]-1,2,3,5-tetrazin-4(3H)-one: a key derivative of antitumor drug temozolomide
AU Wang, Yongfeng; Stevens, Malcolm F. G.
CS Cancer Res. Campaign Experimental Cancer Chemotherapy Res. Group, Univ. Nottingham, Nottingham, NG7 2RD, UK
SO Bioorg. Med. Chem. Lett. (1996), 6(2), 185-8
CODEN: BMCLE8; ISSN: 0960-894X
DT Journal
LA English
OS CASREACT 124:232405

V. Balasubramanian

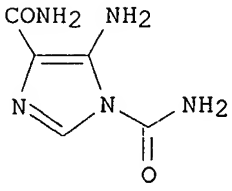
GI



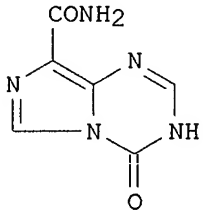
I



II



III



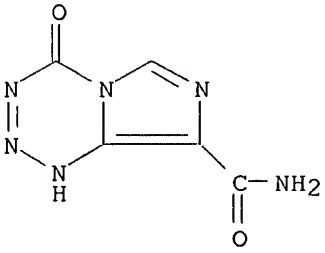
IV

AB 5-Diazoimidazole-4-carboxamide (I) reacted with trimethylsilyl isocyanate in acetonitrile to afford 8-carbamoylimidazo[5,1-d]1,2,3,5-tetrazin-4(3H)-one (II; R = H), which was undergoing a methylation to give antitumor drug temozolomide (II; R = Me); while 1,5-dicarbamoylaminoimidazole (III) failed in an azo-cyclization to give II (R = H) but accomplished a carbon-cyclization to produce 8-carbamoylimidazo[1,5-a] s-triazin-4(3H)-one (IV).

IT **108030-65-5P**, Nortemozolomide
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**
(synthetic studies with carbamoylimidazotetrazinone)

RN 108030-65-5 CAPLUS

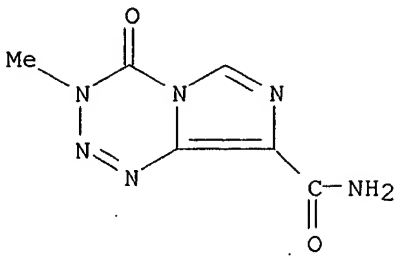
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



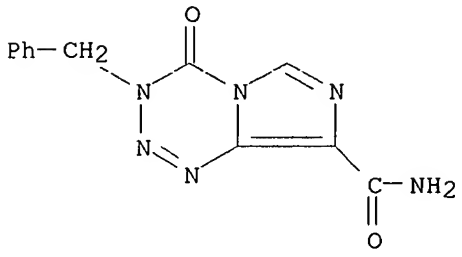
IT **85622-93-1P**, Temozolomide **85623-02-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(synthetic studies with carbamoylimidazotetrazinone)

RN 85622-93-1 CAPLUS

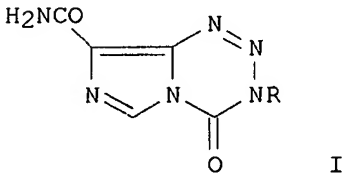
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



RN 85623-02-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1995:933775 CAPLUS
DN 124:117266
TI Antitumor imidazotetrazines. Part 33. New syntheses of the antitumor drug temozolomide using 'masked' methyl isocyanates
AU Wang, Yongfeng; Stevens, Malcolm F. G.; Thomson, William T.; Shutts, Bruce P.
CS Cancer Res. Lab., Dep. Pharmaceutical Sci., Univ. Nottingham, Nottingham, NG7 2RD, UK
SO J. Chem. Soc., Perkin Trans. 1 (1995), (21), 2783-7
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 124:117266
GI



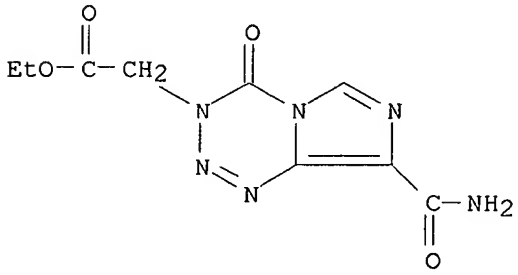
I

AB The imidazotetrazinylacetate I [R = CH2CO2Et] can be prepd. by treating 5-diazoimidazole-4-carboxamide with Et isocyanatoacetate or by diazotization of N-(5-amino-4-carbamoylimidazol-1-ylcarbonyl)glycine Et ester. Hydrolysis to the acid and Barton radical decarboxylation affords

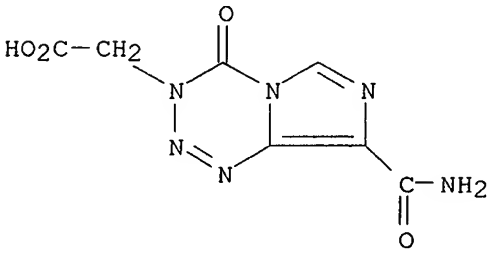
temozolomide (II) (26%) whereas deprotection of I [R = CH2SiMe3] with TBAF in acetonitrile-acetic acid gives 78% II. I [R = CH2Ph, CH2C6H4OMe-4, CHPh2] are stable to hydrogenolytic or oxidative debenzylation reactions.

IT **157466-97-2P 157466-98-3P 157466-99-4P**
157467-00-0P 172988-50-0P 172988-51-1P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**
(Preparation)
(prepn. of temozolomide and related imidazotetrazines using masked Me isocyanates)

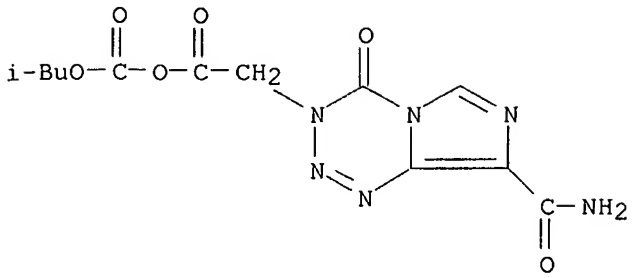
RN 157466-97-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-3(4H)-acetic acid, 8-(aminocarbonyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



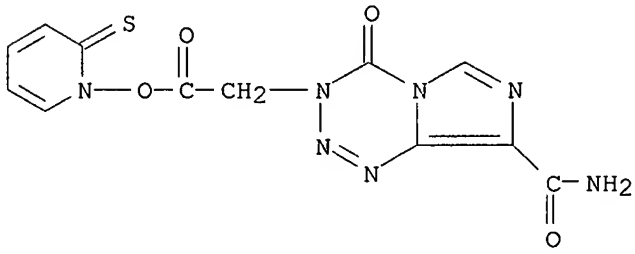
RN 157466-98-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-3(4H)-acetic acid, 8-(aminocarbonyl)-4-oxo- (9CI) (CA INDEX NAME)



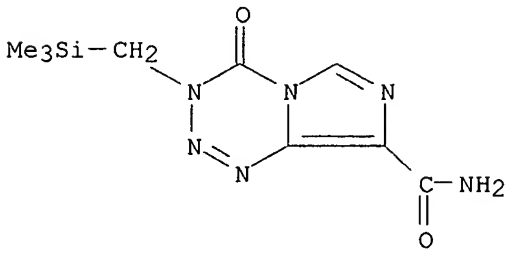
RN 157466-99-4 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-3(4H)-acetic acid, 8-(aminocarbonyl)-4-oxo-, anhydride with 2-methylpropyl hydrogen carbonate (9CI) (CA INDEX NAME)



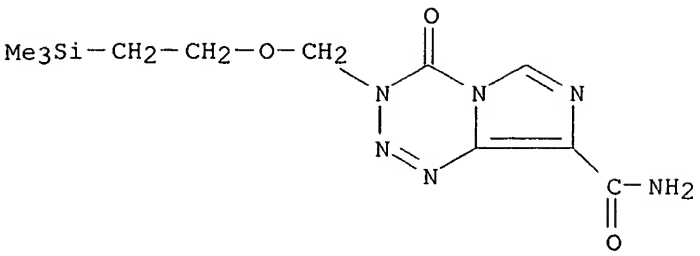
RN 157467-00-0 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-[2-oxo-2-[(2-thioxo-1(2H)-pyridinyl)oxy]ethyl]- (9CI) (CA INDEX NAME)



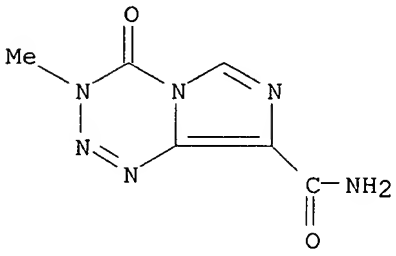
RN 172988-50-0 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-[(trimethylsilyl)methyl]- (9CI) (CA INDEX NAME)



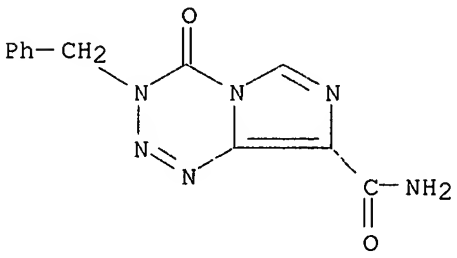
RN 172988-51-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-[[2-(trimethylsilyl)ethoxy]methyl]- (9CI) (CA INDEX NAME)



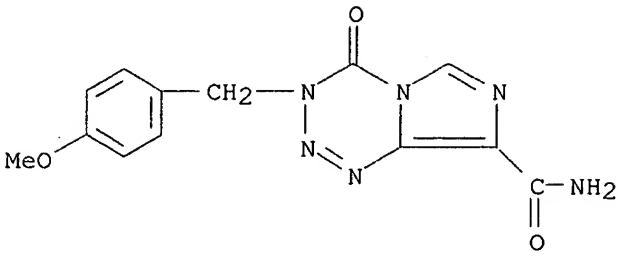
IT **85622-93-1P**, Temozolomide **85623-02-5P**
85623-05-8P 172988-48-6P 172988-49-7P
172988-52-2P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of temozolomide and related imidazotetrazines using masked Me isocyanates)
RN 85622-93-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



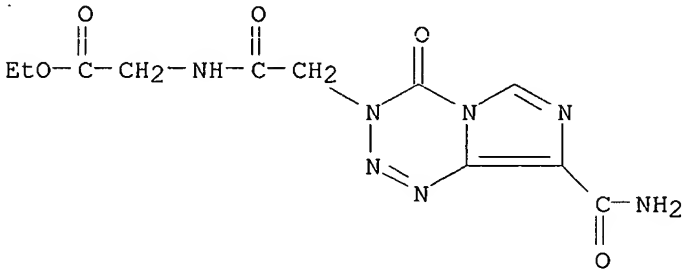
RN 85623-02-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



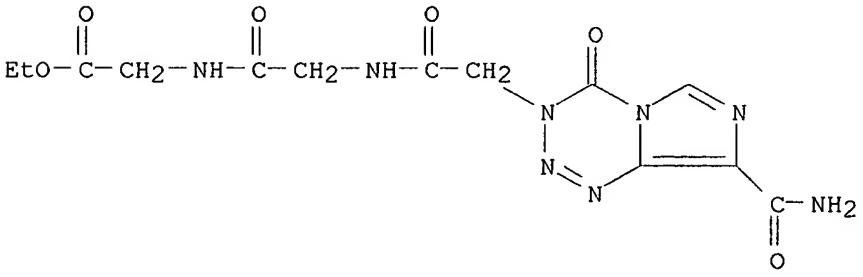
RN 85623-05-8 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-[(4-methoxyphenyl)methyl]-4-oxo- (9CI) (CA INDEX NAME)



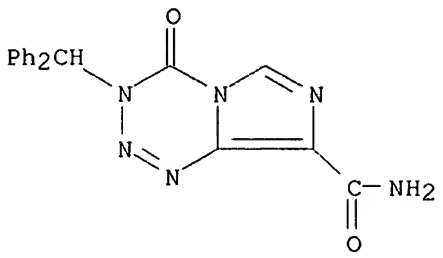
RN 172988-48-6 CAPLUS
CN Glycine, N-[[8-(aminocarbonyl)-4-oxoimidazo[5,1-d]-1,2,3,5-tetrazin-3(4H)-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



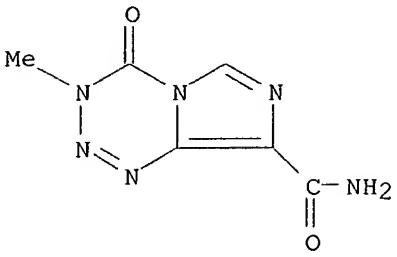
RN 172988-49-7 CAPLUS
CN Glycine, N-[[[8-(aminocarbonyl)-4-oxoimidazo[5,1-d]-1,2,3,5-tetrazin-3(4H)-yl]acetyl]glycyl]-, ethyl ester (9CI) (CA INDEX NAME)



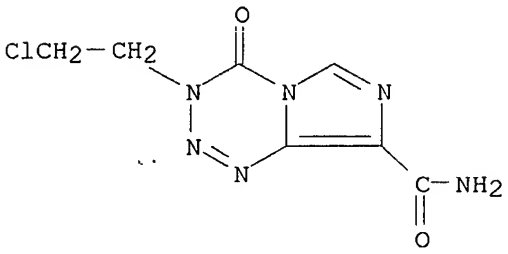
RN 172988-52-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(diphenylmethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



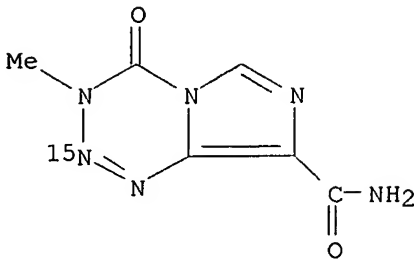
L6 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1995:508250 CAPLUS
DN 123:198751
TI Antitumor Imidazotetrazines. 32.1 Synthesis of Novel Imidazotetrazinones and Related Bicyclic Heterocycles To Probe the Mode of Action of the Antitumor Drug Temozolomide
AU Clark, A. S.; Deans, B.; Stevens, M. F. G.; Tisdale, M. J.; Wheelhouse, R. T.; Denny, B. J.; Hartley, J. A.
CS Pharmaceutical Sciences Institute, Aston University, Birmingham, B4 7ET, UK
SO J. Med. Chem. (1995), 38(9), 1493-504
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB A series of new imidazo[5,1-d]-1,2,3,5-tetrazinones with addnl. hydrogen-bonding or ionic substituents at the 8-carboxamide position of the antitumor drugs temozolomide and mitozolomide were prepd. None of these compds. were significantly more cytotoxic in vitro against the mouse TLX5 lymphoma than the lead structures. Mol. modeling techniques were used to design benzo- and pyrazolo[4,3-d]-1,2,3-triazinones bearing carboxamide groups in appropriate positions which are isosteric with temozolomide and mitozolomide but which cannot ring open to alkylating species. As predicted, these compds. have no inhibitory properties against human GM892A or Raji cell lines in vitro. Temozolomide and the spermidine-temozolomide conjugate 28 preferentially methylate guanines within guanine-rich sequences in DNA, but no exptl. evidence has been found to support the hypothesis that such regions are involved in catalyzing the ring opening of the imidazotetrazinone prodrugs to their active forms.
IT **85622-93-1DP**, Temozolomide, derivs. **85622-95-3DP**, Mitozolomide, derivs.
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**
(prepn. of imidazotetrazinones as probes for action of temozolomide)
RN 85622-93-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



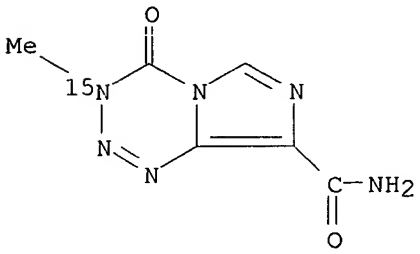
RN 85622-95-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



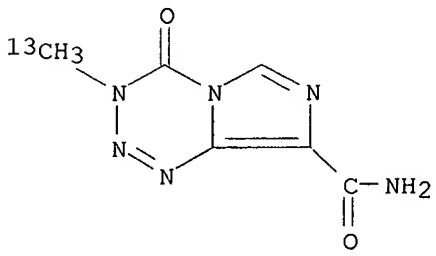
L6 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1995:374136 CAPLUS
DN 122:214043
TI Antitumor imidazotetrazines. Part 31. The synthesis of isotopically labeled temozolomide and a multinuclear (1H, 13C, 15N) magnetic resonance investigation of temozolomide and mitozolomide
AU Wheelhouse, Richard T.; Wilman, Derry E. V.; Thomson, William; Stevens, Malcolm F. G.
CS Cancer Res. Laboratories, Univ. Nottingham, Nottingham, NG7 2RD, UK
SO J. Chem. Soc., Perkin Trans. 1 (1995), (3), 249-52
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 122:214043
AB The antitumor drug temozolomide has been synthesized isotopically labeled with NMR active nuclei at a variety of sites and all its 13C and 15N NMR spectral resonances have been assigned. At low pH a site of protonation has been identified which accounts for the acid stability of the drug.
IT **162021-24-1P 162021-28-5P 162021-29-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(synthesis of isotopically labeled temozolomide and a multinuclear magnetic resonance investigation of temozolomide and mitozolomide)
RN 162021-24-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-2-15N-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



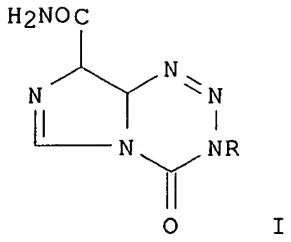
RN 162021-28-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-3-15N-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



RN 162021-29-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(methyl-13C)-4-oxo- (9CI) (CA INDEX NAME)



L6 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1994:557614 CAPLUS
DN 121:157614
TI Alternative syntheses of the antitumor drug temozolomide avoiding the use of methyl isocyanate
AU Wang, Yongfeng; Stevens, Malcolm F. G.; Thomson, W.
CS Cancer Res. Lab., Univ. Nottingham, Nottingham, NG7 2RD, UK
SO J. Chem. Soc., Chem. Commun. (1994), (14), 1687-8
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 121:157614
GI



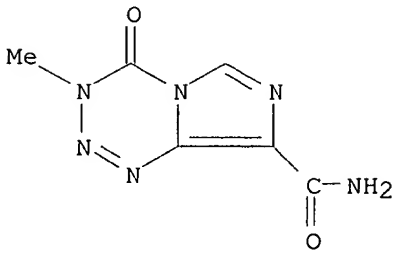
I

AB Et (8-carbamoyl-3,4-dihydro-4-oxoimidazo[5,1-d]-1,2,3,5-tetrazin-3-yl)acetate (I, R = CH2CO2Et) can be prepd. by two routes starting from 5-aminoimidazole-4-carboxamide; hydrolysis of I (R = CH2CO2Et) to the corresponding carboxylic acid followed by Barton radical decarboxylation gives the antitumor imidazotetrazinone temozolomide (I, R = Me).

IT **85622-93-1P,** Temozolomide
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(alternative synthesis of)

RN 85622-93-1 CAPLUS

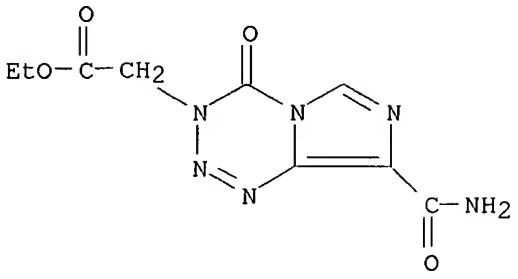
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



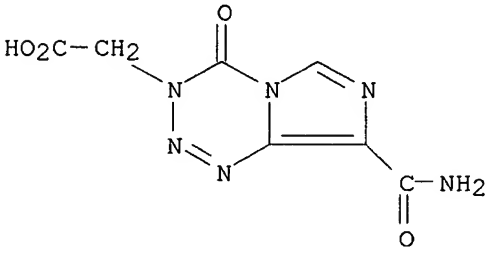
IT **157466-97-2P 157466-98-3P 157466-99-4P**
157467-00-0P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and reaction of, in synthesis of temozolomide)

RN 157466-97-2 CAPLUS

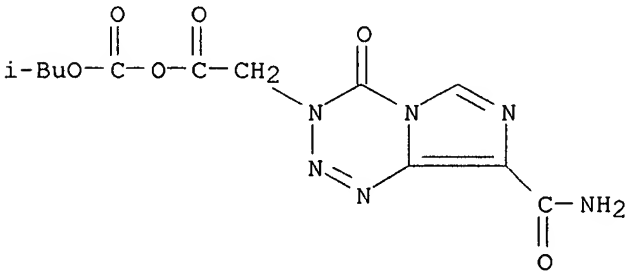
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-3(4H)-acetic acid, 8-(aminocarbonyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



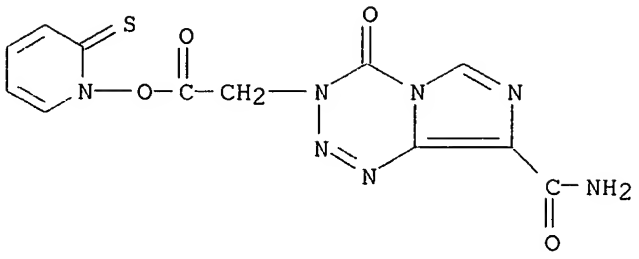
RN 157466-98-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-3(4H)-acetic acid, 8-(aminocarbonyl)-4-oxo- (9CI) (CA INDEX NAME)



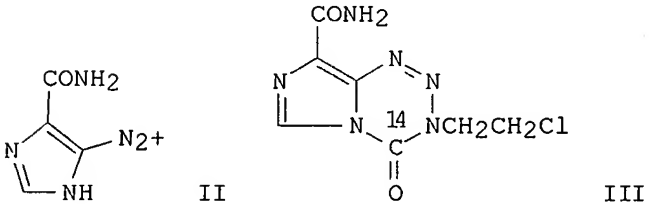
RN 157466-99-4 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-3(4H)-acetic acid, 8-(aminocarbonyl)-4-oxo-, anhydride with 2-methylpropyl hydrogen carbonate (9CI) (CA INDEX NAME)



RN 157467-00-0 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-[2-oxo-2-[(2-thioxo-1(2H)-pyridinyl)oxy]ethyl]- (9CI) (CA INDEX NAME)

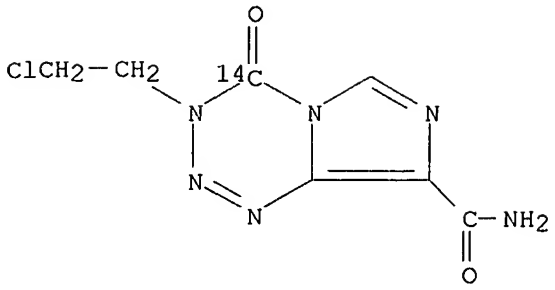


L6 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1989:94466 CAPLUS
DN 110:94466
TI Carbon-14 labeling of 2-chloroethyl isocyanate. Application to the labeling of (chloroethyl)tetrazinone and (chloroethyl)nitrosoureas
AU Madelmont, J. C.; Moreau, M. F.; Godeneche, D.; Labarre, P.; Veyre, A.
CS INSERM, Clermont-Ferrand, 63005, Fr.
SO J. Labelled Compd. Radiopharm. (1988), 25(10), 1135-42
CODEN: JLCRD4; ISSN: 0362-4803
DT Journal
LA French
OS CASREACT 110:94466
GI

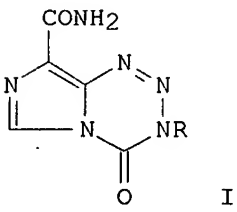


II III

AB Isocyanate ClCH2CH2N14CO (I) was prepd. from ClCH2CH214CO2H via the acyl azide. I was converted to an aryl carbamate, and subsequent nitrosation, amidation (MeSCH2CH2NH2), and oxidn. gave ureas MeS(O)nCH2CH2NH14CON(NO)CH2CH2Cl (n = 1, 2). The reaction of I with imidazolediazonium compd. II gave 14C-labeled mitozolomide (III).
IT **118971-95-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 118971-95-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-4-14C-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L6 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1988:68357 CAPLUS
DN 108:68357
TI Antitumor activity and pharmacokinetics in mice of 8-carbamoyl-3-methylimidazo[5,1-d]-1,2,3,5-tetrazin-4(3H)-one (CCRG 81045; M & B 39831), a novel drug with potential as an alternative to dacarbazine
AU Stevens, Malcolm F. G.; Hickman, John A.; Langdon, Simon P.; Chubb, David; Vickers, Lisa; Stone, Robert; Baig, Ghousia; Goddard, Colin; Gibson, Neil W.; et al.
CS Pharm. Sci. Inst., Aston Univ., Birmingham, B4 7ET, UK
SO Cancer Res. (1987), 47(22), 5846-52
CODEN: CNREA8; ISSN: 0008-5472
DT Journal
LA English
GI



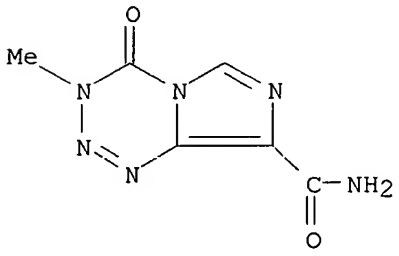
I

AB A no. of 3-alkyl analogs [I, e.g., R = Me, Et, (CH2)2Br, or Pr] of the exptl. antitumor drug mitozolomide [I, R = (CH2)2Cl] were screened against murine tumors in vivo. Only the compds. with a 3-methyl- or 3-bromoethyl group had significant antitumor activity against the TLX5 lymphoma. The 3-Me analog, CCRG 81045 (II) had good activity, when administered i.p., against L1210 and P388 leukemias, M5076 reticulum cell sarcoma, B16 melanoma, and ADJ/PC6A plasmacytoma. II was also active when administered orally to mice bearing the L1210 leukemia. A daily schedule of 100 mg/kg II for 5 days produced increases of survival time of treated animals compared to controls of 176 and >235% against the P388 and L1210 leukemias, resp. In the female C57BL .times. DBA/2 F1 mouse the 10% LD was 125 mg/kg daily for 5 days. II underwent mild alk. hydrolysis and ring fission to form the linear triazene, 5-(3-methyltriazen-1-yl)imidazole-4-carboxamide (III), which is the putative metabolite formed upon metabolic activation of the antitumor drug dacarbazine [5-(3,3-dimethyltriazen-1-yl)imidazole-4-carboxamide]. The half-life of II at 37.degree. in 0.2M phosphate buffer (pH 7.4) was 1.24 h, whereas

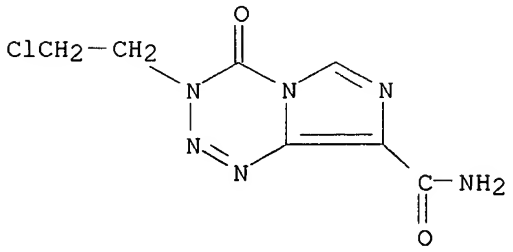
that of III at 25.degree. was 8 min. The half-life of II in human plasma in vitro at 37.degree. was 0.42 h. Pharmacokinetic expts. conducted in BALB/c mice produced plasma profiles of II, administered i.p. or orally, which showed a rapid absorption phase, elimination half-lives of 1.13 h (i.p.) and 1.29 h (oral) and a bioavailability of 0.98.

IT **85622-93-1P**, CCRG 81045 **85622-95-3P**, Mitozolomide
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and antitumor activity and pharmacokinetics of)

RN 85622-93-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)

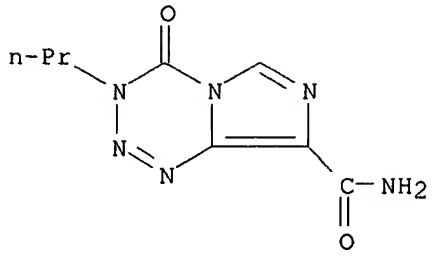


RN 85622-95-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

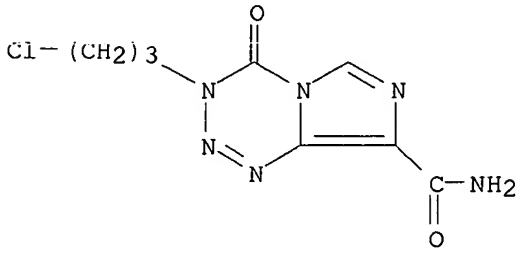


IT **85622-94-2P 85622-97-5P 85622-98-6P**
85622-99-7P 85623-01-4P 85623-02-5P
85623-03-6P 97716-74-0P 108030-65-5DP, derivs.
112557-08-1P 112557-09-2P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. and antitumor activity of)

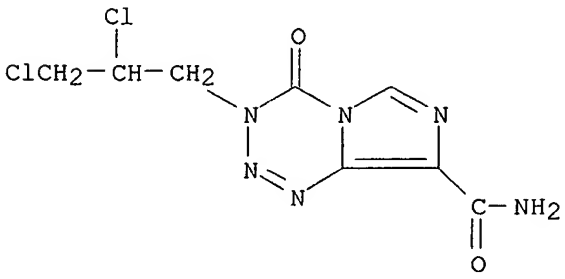
RN 85622-94-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-propyl- (9CI) (CA INDEX NAME)



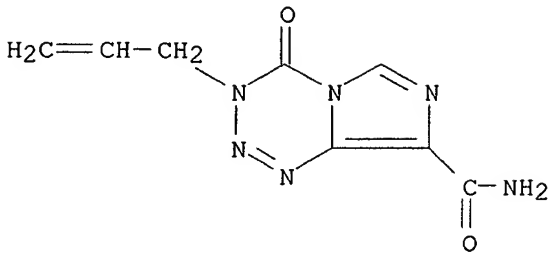
RN 85622-97-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(3-chloropropyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



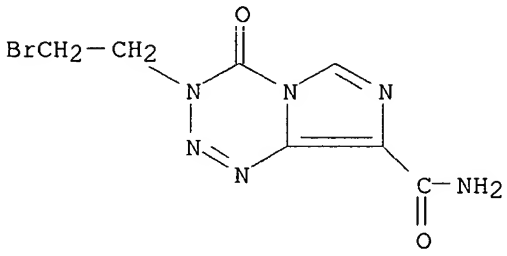
RN 85622-98-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2,3-dichloropropyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



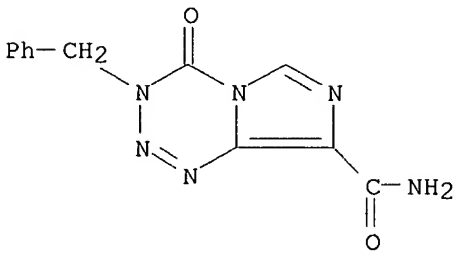
RN 85622-99-7 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(2-propenyl)- (9CI) (CA INDEX NAME)



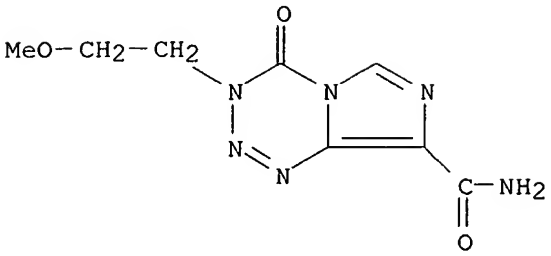
RN 85623-01-4 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-bromoethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



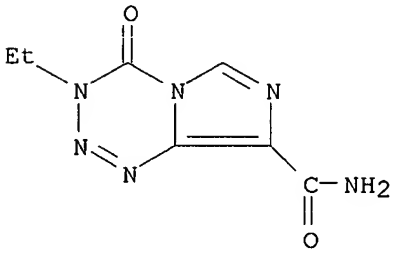
RN 85623-02-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



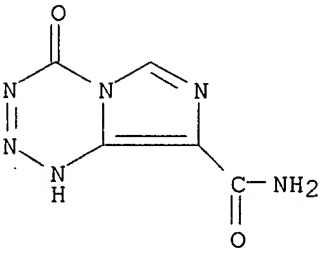
RN 85623-03-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(2-methoxyethyl)-4-oxo- (9CI) (CA INDEX NAME)



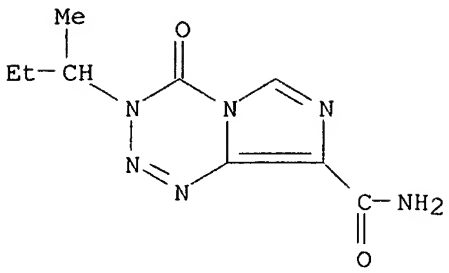
RN 97716-74-0 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-ethyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



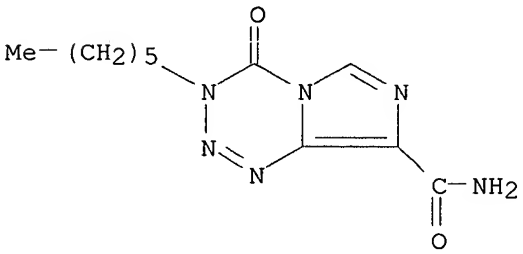
RN 108030-65-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



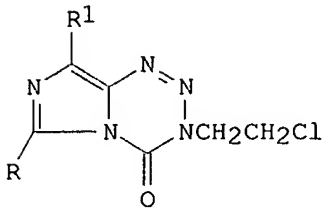
RN 112557-08-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(1-methylpropyl)-4-oxo- (9CI) (CA INDEX NAME)



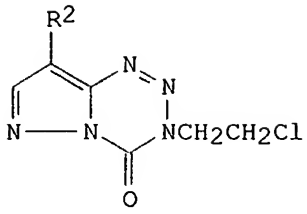
RN 112557-09-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-hexyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



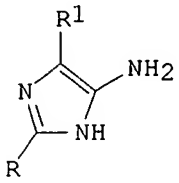
L6 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1987:102242 CAPLUS
DN 106:102242
TI Antitumor imidazotetrazines. 14. Synthesis and antitumor activity of 6- and 8-substituted imidazo[5,1-d]-1,2,3,5-tetrazinones and 8-substituted pyrazolo[5,1-d]-1,2,3,5-tetrazinones
AU Lunt, Edward; Newton, Christopher G.; Smith, Christopher; Stevens, Graham P.; Stevens, Malcolm F. G.; Straw, Colin G.; Walsh, Roger J. A.; Warren, Peter J.; Fizames, Christian; et al.
CS Res. Inst., May and Baker Ltd., Dagenham/Essex, RM10 7XS, UK
SO J. Med. Chem. (1987), 30(2), 357-66
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 106:102242
GI



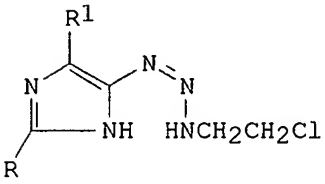
I



II



IV



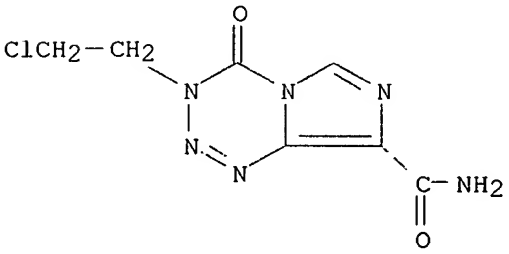
V

AB Imidazo[5,1-d]-1,2,3,5-tetrazinones I (R = alkyl or aralkyl, R1 = CONH2; R = H, R1 = CONHMe, CONMe2, CN, SO2Me, SO2NHMe, etc.) and pyrazolo[5,1-d]-1,2,3,5-tetrazinones II (R2 = CONH2, CONMe2, NO2, SO2Me) were prepd. as derivs. of the antitumor agent mitozolomide (I; R = H, R1 = CONH2) (III). Thus, imidazoles IV were diazotized and the cyclized with ClCH2CH2NCO to give the corresponding I. I (R = alkyl or aralkyl, R1 = CONH2) showed optimal antitumor activity when the group was small or linear, but activity diminished as size and branching of this substituent increased. This may reflect altered transport characteristics, or failure of the enlarged derivs. to fit a binding site, or possibly a reduced tendency for the derivs. having bulky groups at position 6 to hydrolytically generate the putatively active triazenes V. Testing of 14 derivs. of III substituted differently at position 8 revealed a complex structure-activity relationship, with good antitumor activity obtained for carbamoyl and sulfamoyl groups bearing small substituents. The 8-methylsulfonyl compd. had noteworthy activity, but the 8-cyano, 8-nitro, and 8-Ph derivs. were devoid of useful antitumor activity.

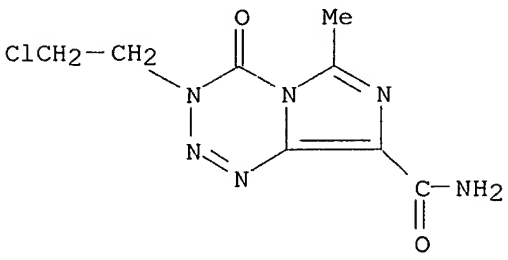
IT **85622-95-3DP**, Mitozolomide, derivs. **90521-16-7P 90521-26-9P 90521-27-0P 90521-28-1P 90521-29-2P 90521-30-5P 90521-31-6P 90521-32-7P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**
(prepn. and antitumor activity of)

RN 85622-95-3 CAPLUS

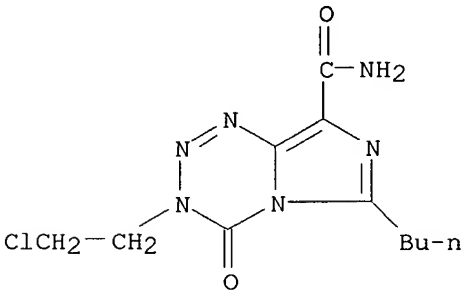
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



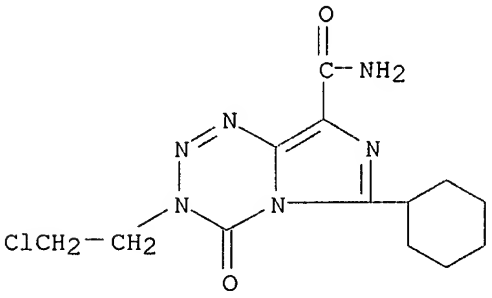
RN 90521-16-7 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-6-methyl-4-oxo- (9CI) (CA INDEX NAME)



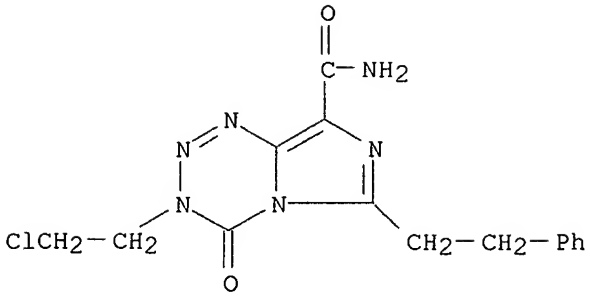
RN 90521-26-9 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 6-butyl-3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



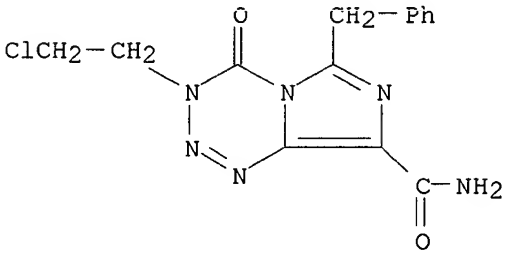
RN 90521-27-0 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-6-cyclohexyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



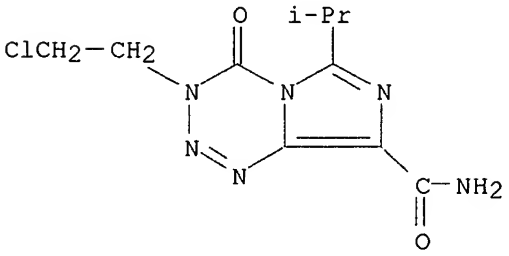
RN 90521-28-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo-6-(2-phenylethyl)- (9CI) (CA INDEX NAME)



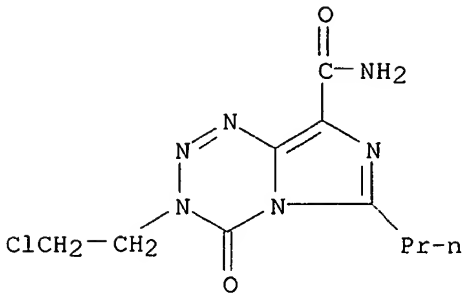
RN 90521-29-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo-6-(phenylmethyl)- (9CI) (CA INDEX NAME)



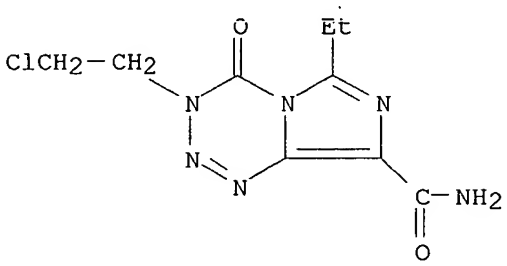
RN 90521-30-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-6-(1-methylethyl)-4-oxo- (9CI) (CA INDEX NAME)



RN 90521-31-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo-6-propyl- (9CI) (CA INDEX NAME)



RN 90521-32-7 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-6-ethyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L6 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1984:423509 CAPLUS
DN 101:23509
TI Tetrazine derivatives
IN Baig, Ghouse Unissa; Stevens, Malcolm Francis Graham; Lunt, Edward; Newton, Christopher Gregory; Pedgrift, Brian Leslie; Smith, Christopher; Straw, Colin Geoffrey; Walsh, Roger John Aitchison; Warren, Peter James
PA May and Baker Ltd., UK
SO Ger. Offen., 74 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

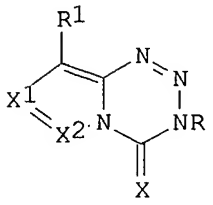
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3329505	A1	19840223	DE 1983-3329505	19830816
	FR 2531958	A1	19840224	FR 1983-13246	19830812
	FR 2531958	B1	19861031		
	SE 8304415	A	19840218	SE 1983-4415	19830815
	SE 455198	B	19880627		
	SE 455198	C	19881006		
	FI 8302927	A	19840218	FI 1983-2927	19830815
	FI 80273	B	19900131		
	FI 80273	C	19900510		
	AU 8317968	A1	19840223	AU 1983-17968	19830815
	AU 575782	B2	19880811		
	GB 2125402	A1	19840307	GB 1983-21942	19830815
	GB 2125402	B2	19851113		

V. Balasubramanian

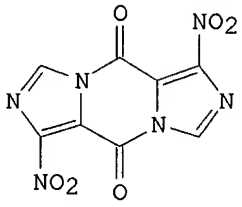
	NL 8302863	A	19840316	NL 1983-2863	19830815
	HU 31735	O	19840528	HU 1983-2860	19830815
	HU 189321	B	19860630		
	ZA 8306003	A	19840725	ZA 1983-6003	19830815
	IL 69500	A1	19890131	IL 1983-69500	19830815
	CA 1254563	A1	19890523	CA 1983-434582	19830815
	DK 8303749	A	19840218	DK 1983-3749	19830816
	AT 8302942	A	19911115	AT 1983-2942	19830816
	BE 897548	A1	19840217	BE 1983-211366	19830817
	JP 59053488	A2	19840328	JP 1983-149273	19830817
	ES 524995	A1	19850101	ES 1983-524995	19830817
	CH 657855	A	19860930	CH 1983-4490	19830817
PRAI	GB 1982-23580		19820817		
	GB 1982-23583		19820817		
	GB 1982-26169		19820914		
	GB 1983-6904		19830314		
	GB 1982-23483		19820817		

OS CASREACT 101:23509

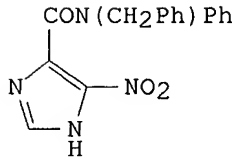
GI



I



II



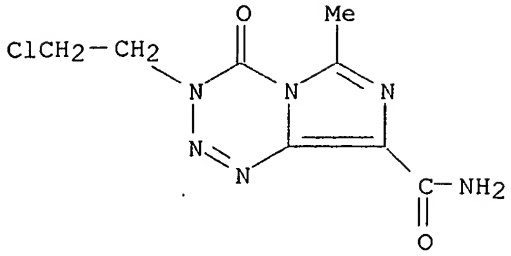
III

AB Antineoplastic (no data) azolotetrazolines I [R = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; R1 = R2S(O)n, sulfamoyl, carbamoyl, acyl, etc.; R2 = alkyl, alkenyl; n = 0-2; X = O, S; X1 or X2 = N, the other = CR3; R3 = H, halo, cyano, OH, NO2, (un)substituted alkyl, alkenyl, Ph, PhO, acyl, etc.] were prepd. Thus, 5-nitro-1H-imidazole-4-carboxylic acid was self-cyclocondensed by heating with PCl5 to give diimidazopyrazinedione II. This was treated with PhCH2NHPh to give imidazolecarboxamide III.HCl, which was hydrogenated to the amine, condensed with NaN3 to give the 5-diazo deriv., and cyclocondensed with MeNCO to give I [R = Me, R1 = CON(CH2Ph)Ph, X, = O, X1 = CH, X2 = N].

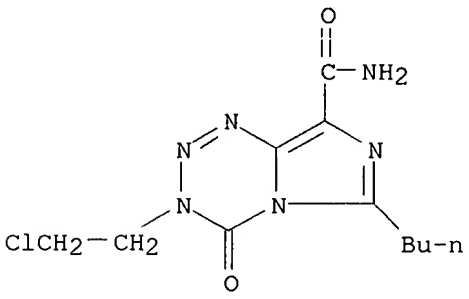
IT **90521-16-7P 90521-26-9P 90521-27-0P**
90521-28-1P 90521-29-2P 90521-30-5P
90521-31-6P 90521-32-7P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

RN 90521-16-7 CAPLUS

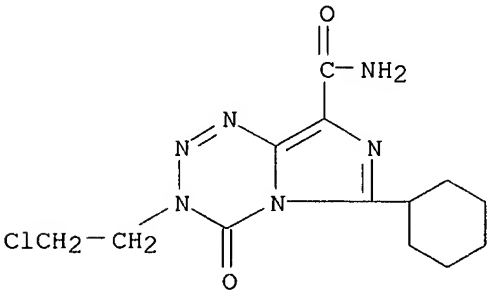
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-6-methyl-4-oxo- (9CI) (CA INDEX NAME)



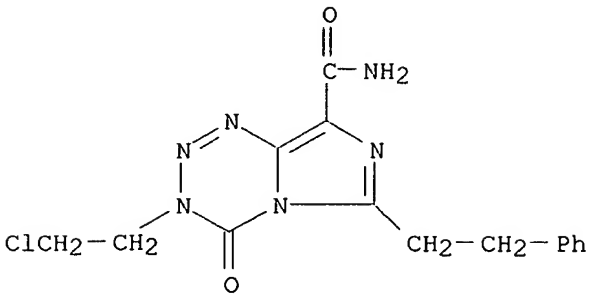
RN 90521-26-9 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 6-butyl-3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



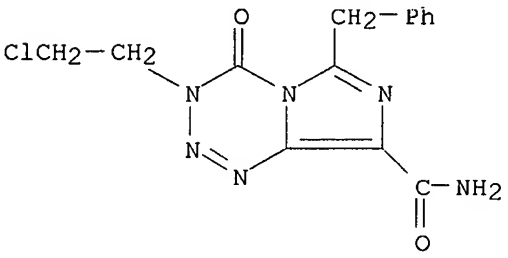
RN 90521-27-0 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-6-cyclohexyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



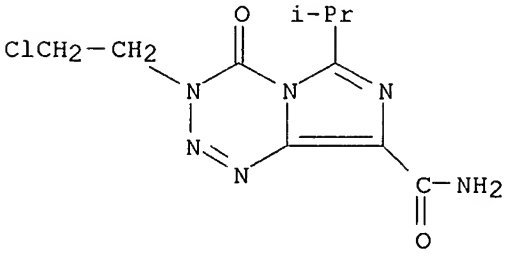
RN 90521-28-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo-6-(2-phenylethyl)- (9CI) (CA INDEX NAME)



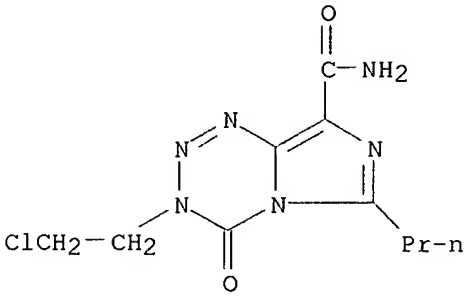
RN 90521-29-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo-6-(phenylmethyl)- (9CI) (CA INDEX NAME)



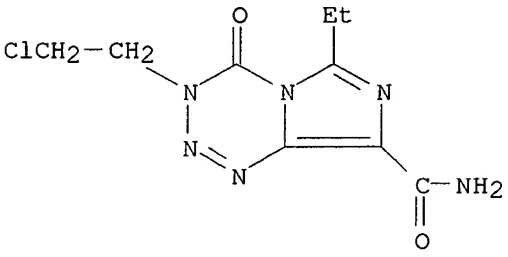
RN 90521-30-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-6-(1-methylethyl)-4-oxo- (9CI) (CA INDEX NAME)



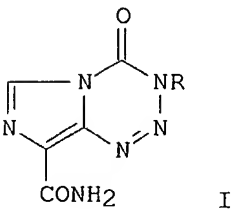
RN 90521-31-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo-6-propyl- (9CI) (CA INDEX NAME)



RN 90521-32-7 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-6-ethyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L6 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1984:51553 CAPLUS
DN 100:51553
TI Antitumour imidazotetrazines. 1. Synthesis and chemistry of 8-carbamoyl-3-(2-chloroethyl)imidazo[5,1-d]-1,2,3,5-tetrazin-4(3H)-one, a novel broad-spectrum antitumor agent
AU Stevens, Malcolm F. G.; Hickman, John A.; Stone, Robert; Gibson, Neil W.; Baig, Ghouse Unissa; Lunt, Edward; Newton, Christopher G.
CS Dep. Pharm., Univ. Aston, Birmingham, B4 7ET, UK
SO J. Med. Chem. (1984), 27(2), 196-201
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



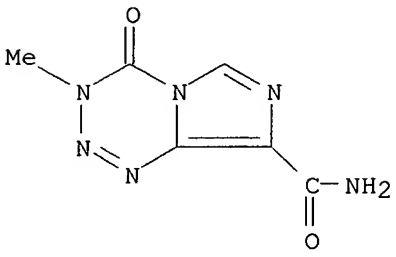
I

AB Interaction of 5-diazo-4-imidazolecarboxamide and alkyl and aryl isocyanates in the dark gave 8-carbamoylimidazo[5,1-d]-1,2,3,5-tetrazin-

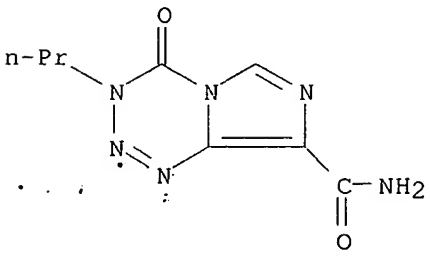
4(3H)-ones (I). In cold MeOH or EtOH, I (R = ClCH2CH2; II) decompd to give 2-azahypoxanthine and ClCH2CH2NHCO2R (R = Me, Et). II was active against L-1210 and P388 leukemia and may act as a prodrug modification of the acyclic triazene 5-[3-(2-chloroethyl)traizen-1-yl]imidazole-4-carboxamide (MCTIC), since it underwent ring opening to form the triazene in aq. Na2CO3.

IT **85622-93-1P 85622-94-2P 87597-51-1P**
87597-52-2P 87597-53-3P 87597-54-4P
87597-55-5P 87597-56-6P 87597-57-7P
87597-58-8P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**
(Preparation)
(prepn. and decompn. of)

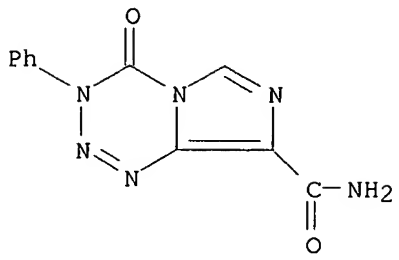
RN 85622-93-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



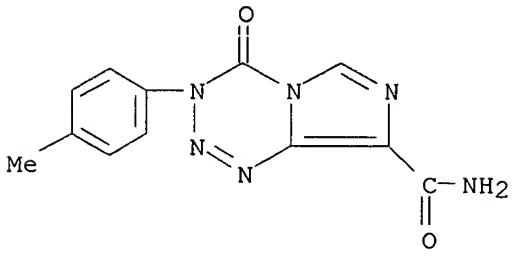
RN 85622-94-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-propyl- (9CI) (CA INDEX NAME)



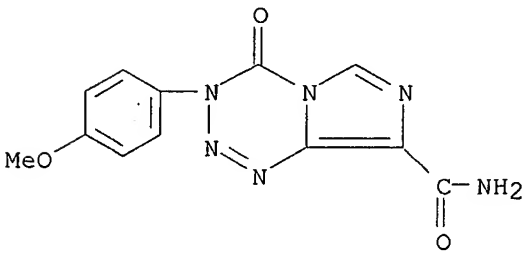
RN 87597-51-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-phenyl- (9CI) (CA INDEX NAME)



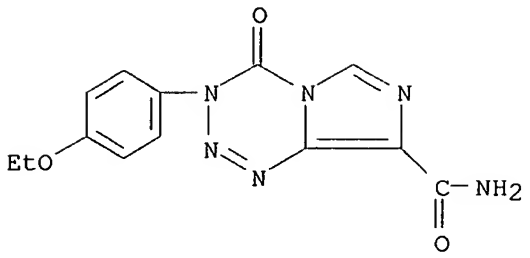
RN 87597-52-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(4-methylphenyl)-4-oxo- (9CI) (CA INDEX NAME)



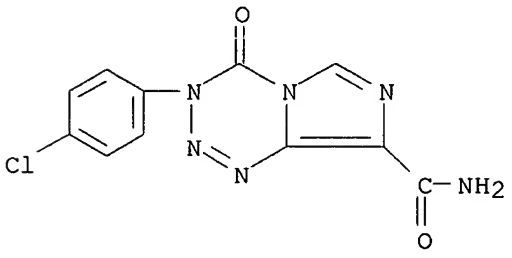
RN 87597-53-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(4-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)



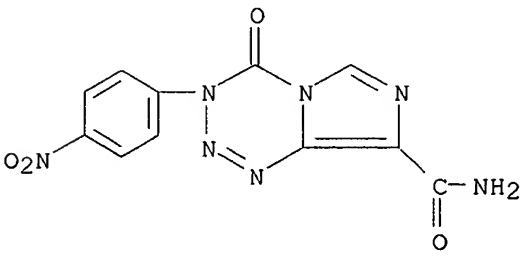
RN 87597-54-4 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(4-ethoxyphenyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



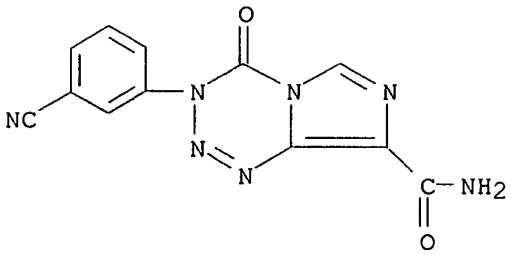
RN 87597-55-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(4-chlorophenyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



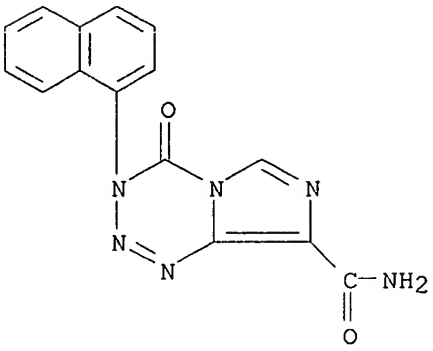
RN 87597-56-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(4-nitrophenyl)-4-oxo- (9CI) (CA INDEX NAME)



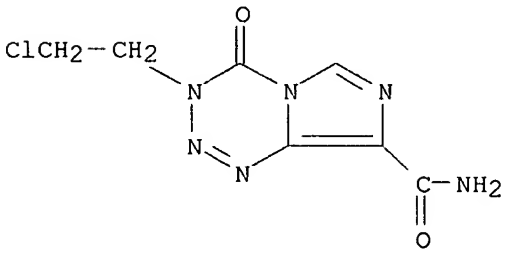
RN 87597-57-7 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(3-cyanophenyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



RN 87597-58-8 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(1-naphthalenyl)-4-oxo- (9CI) (CA INDEX NAME)



IT **85622-95-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**
(prepn., degrdn., and antitumor activity of)
RN 85622-95-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



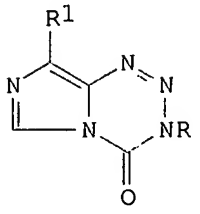
L6 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1983:198285 CAPLUS
DN 98:198285
TI Tetrazine derivatives and pharmaceutical compositions containing them
IN Lunt, Edward; Stevens, Malcolm Francis Graham; Stone, Robert; Wooldridge, Kenneth Robert Harry

V. Balasubramanian

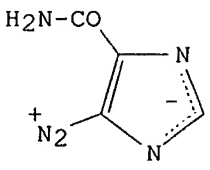
PA May and Baker Ltd., UK
SO Ger. Offen., 29 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3231255	A1	19830303	DE 1982-3231255	19820823
	DE 3231255	C2	19920227		
	IL 66606	A1	19870731	IL 1982-66606	19820812
	BE 894175	A1	19830223	BE 1982-208860	19820823
	DK 8203778	A	19830225	DK 1982-3778	19820823
	DK 161147	B	19910603		
	DK 161147	C	19911118		
	FI 8202921	A	19830225	FI 1982-2921	19820823
	FI 73434	B	19870630		
	FI 73434	C	19871009		
	FR 2511679	A1	19830225	FR 1982-14461	19820823
	FR 2511679	B1	19850201		
	SE 8204817	A	19830225	SE 1982-4817	19820823
	SE 448543	B	19870302		
	SE 448543	C	19870611		
	AU 8287493	A1	19830303	AU 1982-87493	19820823
	AU 571430	B2	19880421		
	GB 2104522	A1	19830309	GB 1982-24155	19820823
	GB 2104522	B2	19850612		
	JP 58043975	A2	19830314	JP 1982-144902	19820823
	JP 04005029	B4	19920130		
	NL 8203286	A	19830316	NL 1982-3286	19820823
	NL 192739	B	19970901		
	NL 192739	C	19980106		
	ZA 8206120	A	19830727	ZA 1982-6120	19820823
	ES 515176	A1	19831101	ES 1982-515176	19820823
	HU 27908	O	19831128	HU 1982-2708	19820823
	HU 186107	B	19850628		
	AT 8203191	A	19850915	AT 1982-3191	19820823
	AT 380256	B	19860512		
	CA 1197247	A1	19851126	CA 1982-409950	19820823
	CH 655114	A	19860327	CH 1982-5007	19820823
	SU 1447284	A3	19881223	SU 1982-3482389	19820823
PRAI	GB 1981-25791	A	19810824		

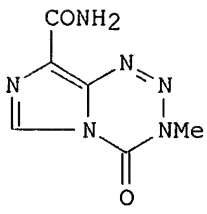
GI



I



II



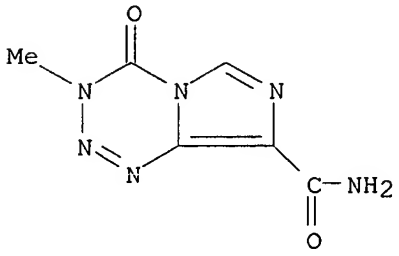
III

AB I [R = (un)substituted H, alkyl, alkenyl, alkynyl, aryl, cycloalkyl; R1 = (un)substituted carbamoyl] were prepd. as antitumor agents (no data). Thus, 500 mg II in 3.0 mL MeNCO were stirred in the dark 21 days to give

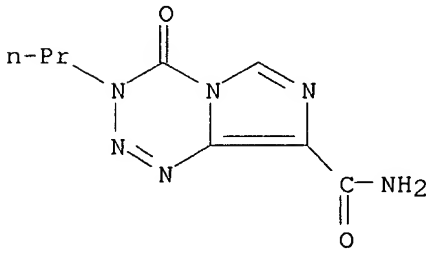
198 mg III.

IT **85622-93-1P 85622-94-2P 85622-95-3P**
85622-97-5P 85622-98-6P 85622-99-7P
85623-01-4P 85623-02-5P 85623-03-6P
85623-04-7P 85623-05-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

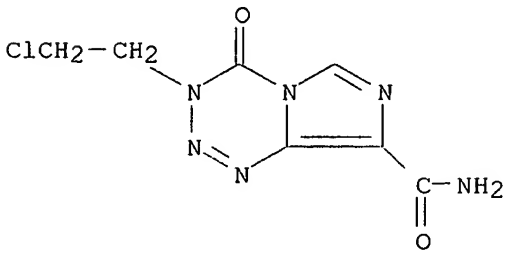
RN 85622-93-1 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



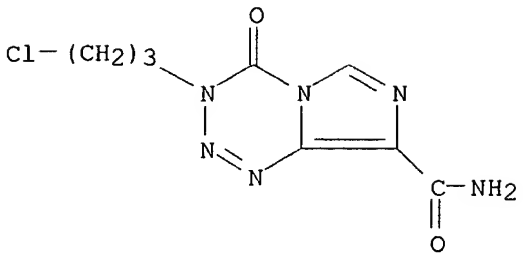
RN 85622-94-2 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-propyl- (9CI) (CA INDEX NAME)



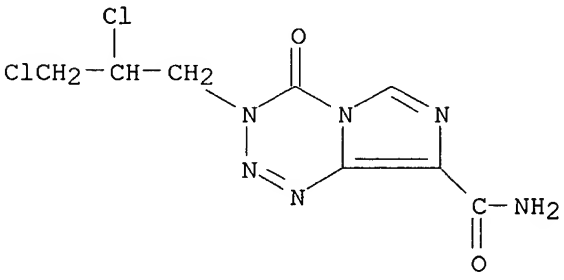
RN 85622-95-3 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



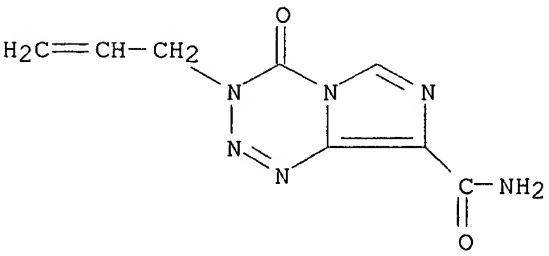
RN 85622-97-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(3-chloropropyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



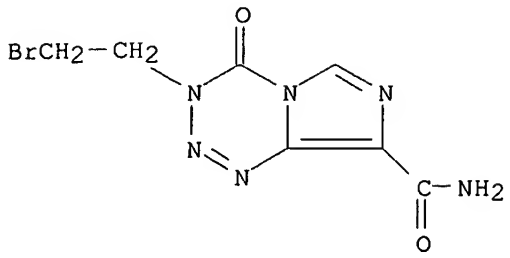
RN 85622-98-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2,3-dichloropropyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



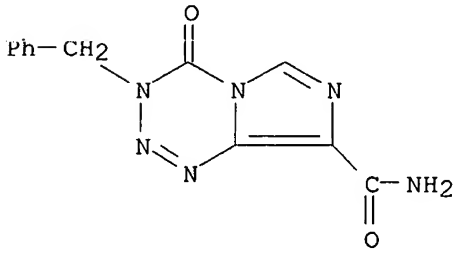
RN 85622-99-7 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(2-propenyl)- (9CI) (CA INDEX NAME)



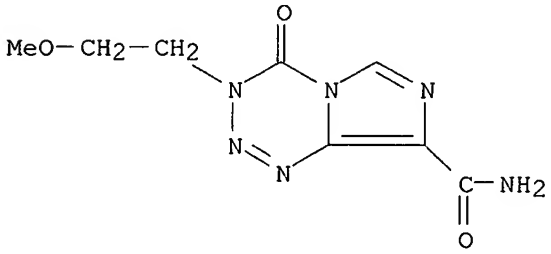
RN 85623-01-4 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-(2-bromoethyl)-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



RN 85623-02-5 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-4-oxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

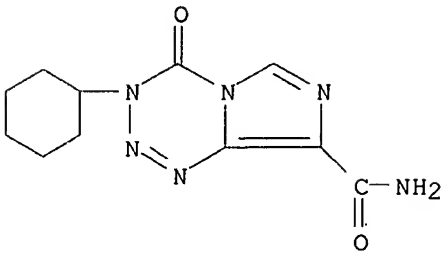


RN 85623-03-6 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-(2-methoxyethyl)-4-oxo- (9CI) (CA INDEX NAME)

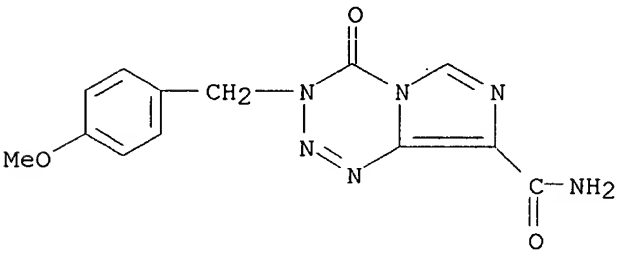


RN 85623-04-7 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3-cyclohexyl-3,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

V. Balasubramanian



RN 85623-05-8 CAPLUS
CN Imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxamide, 3,4-dihydro-3-[(4-methoxyphenyl)methyl]-4-oxo- (9CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	77.43	220.20

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-10.53	-10.53

STN INTERNATIONAL LOGOFF AT 16:30:29 ON 06 MAY 2002

Welcome to STN International! Enter x:x

LOGINID:ssspta1611bxv

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	Jan 25	BLAST(R) searching in REGISTRY available in STN on the Web
NEWS	3	Jan 29	FSTA has been reloaded and moves to weekly updates
NEWS	4	Feb 01	DKILIT now produced by FIZ Karlsruhe and has a new update

```
                    frequency
 NEWS  5   Feb 19   Access via Tymnet and SprintNet Eliminated Effective 3/31/02
 NEWS  6   Mar 08   Gene Names now available in BIOSIS
 NEWS  7   Mar 22   TOXLIT no longer available
 NEWS  8   Mar 22   TRCTHERMO no longer available
 NEWS  9   Mar 28   US Provisional Priorities searched with P in CA/CAplus
                    and USPATFULL
 NEWS 10   Mar 28   LIPINSKI/CALC added for property searching in REGISTRY
 NEWS 11   Apr 02   PAPERCHEM no longer available on STN.  Use PAPERCHEM2 instead.
 NEWS 12   Apr 08   "Ask CAS" for self-help around the clock
 NEWS 13   Apr 09   BEILSTEIN: Reload and Implementation of a New Subject Area
 NEWS 14   Apr 09   ZDB will be removed from STN
 NEWS 15   Apr 19   US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
 NEWS 16   Apr 22   Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
 NEWS 17   Apr 22   BIOSIS Gene Names now available in TOXCENTER
 NEWS 18   Apr 22   Federal Research in Progress (FEDRIP) now available
 NEWS 19   May 31   PCTFULL to be reloaded.  File temporarily unavailable.

 NEWS EXPRESS  February 1 CURRENT WINDOWS VERSION IS V6.0d,
               CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
               AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *



FILE 'HOME' ENTERED AT 12:54:48 ON 03 JUN 2002

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.21       0.21

FILE 'REGISTRY' ENTERED AT 12:54:56 ON 03 JUN 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:    2 JUN 2002  HIGHEST RN 424787-52-0
DICTIONARY FILE UPDATES:   2 JUN 2002  HIGHEST RN 424787-52-0

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002
```

V. Balasubramanian

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

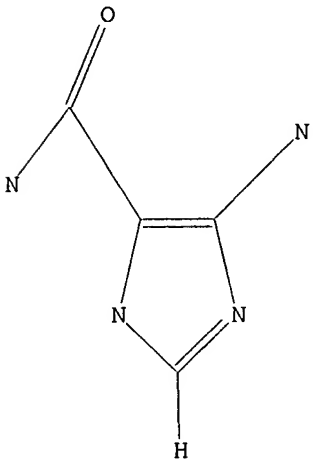
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10050488.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 12:55:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 138 TO ITERATE

100.0% PROCESSED 138 ITERATIONS 44 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2056 TO 3464
PROJECTED ANSWERS: 483 TO 1277

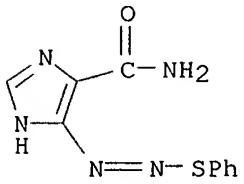
L2 44 SEA SSS SAM L1

=> d scan

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-[(phenylthio)azo]- (9CI)

V. Balasubramanian

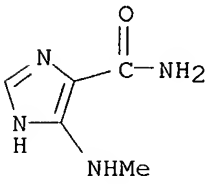
MF C10 H9 N5 O S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

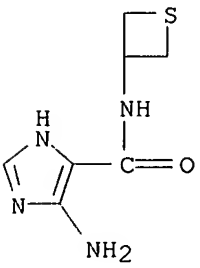
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):43

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-(methylamino)- (9CI)
MF C5 H8 N4 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-amino-N-3-thietanyl- (9CI)
MF C7 H10 N4 O S

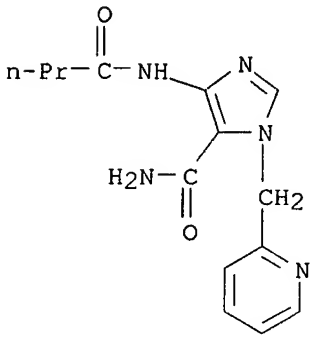


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-[(1-oxobutyl)amino]-1-(2-pyridinylmethyl)-

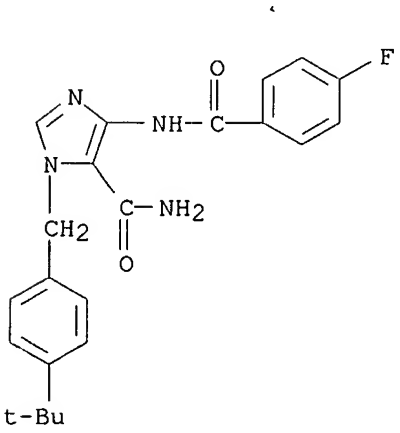
V. Balasubramanian

(9CI)
MF C14 H17 N5 O2



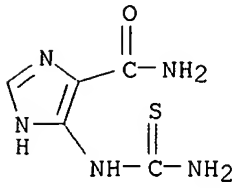
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 1-[[4-(1,1-dimethylethyl)phenyl]methyl]-4-[(4-fluorobenzoyl)amino]- (9CI)
MF C22 H23 F N4 O2



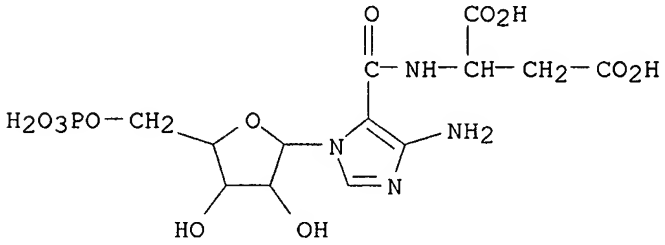
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Urea, 1-(5-carbamoylimidazol-4-yl)-2-thio- (8CI)
MF C5 H7 N5 O S



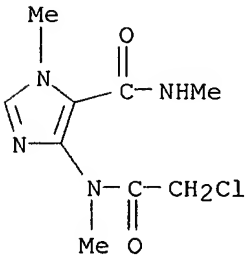
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Aspartic acid, N-[(5-amino-1-ribofuranosylimidazol-4-yl)carbonyl]-, mono(dihydrogen phosphate) (ester), L- (8CI)
MF C13 H19 N4 O12 P



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-[(chloroacetyl)methylamino]-N,1-dimethyl- (9CI)
MF C9 H13 Cl N4 O2

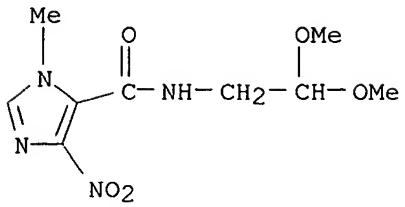


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, N-(2,2-dimethoxyethyl)-1-methyl-4-nitro- (9CI)

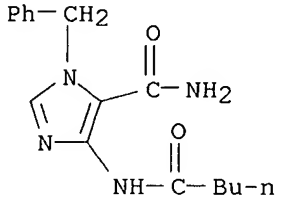
V. Balasubramanian

MF C9 H14 N4 O5



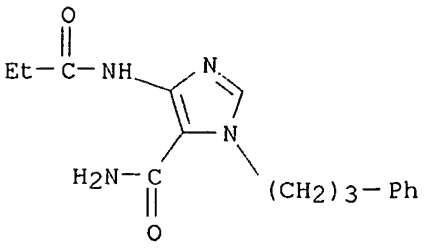
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-[(1-oxopentyl)amino]-1-(phenylmethyl)- (9CI)
MF C16 H20 N4 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-[(1-oxopropyl)amino]-1-(3-phenylpropyl)-
(9CI)
MF C16 H20 N4 O2

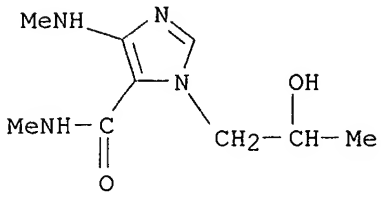


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS

V. Balasubramanian

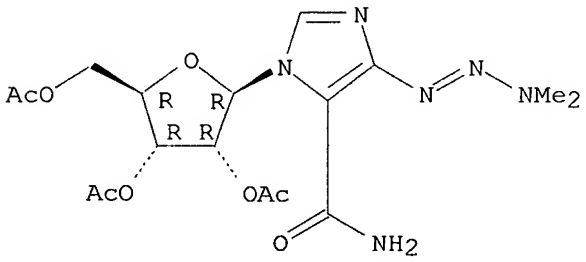
IN 1H-Imidazole-5-carboxamide, 1-(2-hydroxypropyl)-N-methyl-4-(methylamino)-
(9CI)
MF C9 H16 N4 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

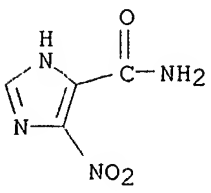
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-(3,3-dimethyl-1-triazenyl)-1-(2,3,5-tri-O-
acetyl-.beta.-D-ribofuranosyl)- (9CI)
MF C17 H24 N6 O8

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-nitro- (9CI)
MF C4 H4 N4 O3

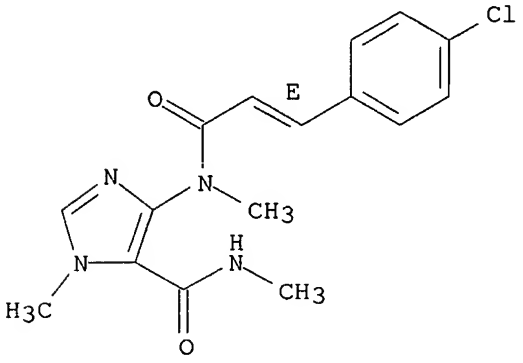


V. Balasubramanian

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

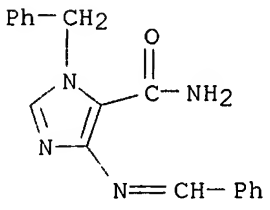
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-[[3-(4-chlorophenyl)-1-oxo-2-propenyl]methylamino]-N,1-dimethyl-, (E)- (9CI)
MF C16 H17 Cl N4 O2

Double bond geometry as shown.



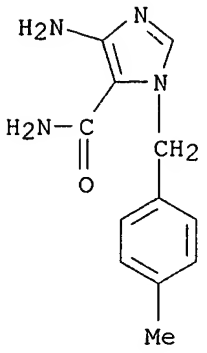
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 1-(phenylmethyl)-4-[(phenylmethylene)amino]- (9CI)
MF C18 H16 N4 O



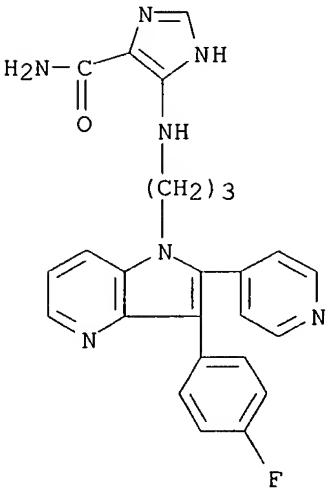
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-amino-1-[(4-methylphenyl)methyl]- (9CI)
MF C12 H14 N4 O



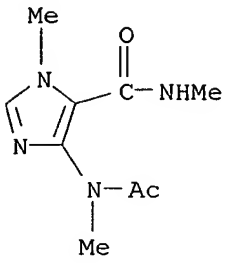
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-[[3-[3-(4-fluorophenyl)-2-(4-pyridinyl)-1H-pyrrolo[3,2-b]pyridin-1-yl]propyl]amino]- (9CI)
MF C25 H22 F N7 O
CI COM



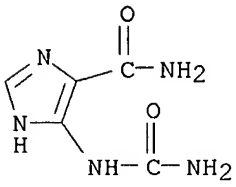
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-(acetylmethylamino)-N,1-dimethyl- (9CI)
MF C9 H14 N4 O2



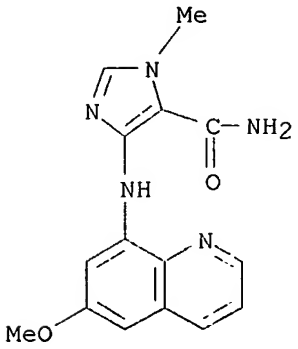
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-[(aminocarbonyl)amino]- (9CI)
MF C5 H7 N5 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

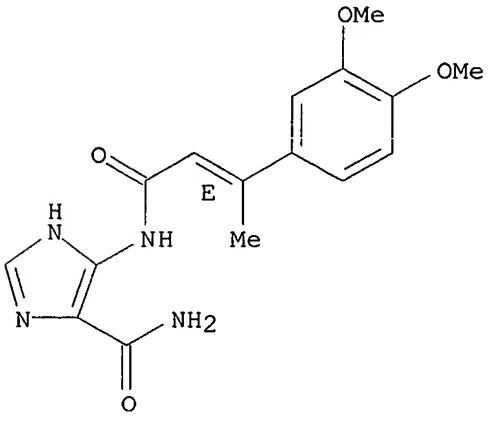
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-[(6-methoxy-8-quinolinyl)amino]-1-methyl-
(9CI)
MF C15 H15 N5 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

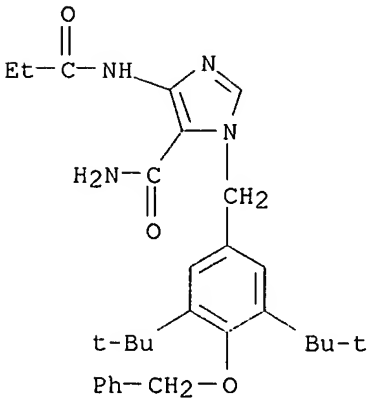
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-[[3-(3,4-dimethoxyphenyl)-1-oxo-2-butenyl]amino]-, monohydrochloride, (E)- (9CI)
MF C16 H18 N4 O4 . Cl H

Double bond geometry as shown.



● HCl

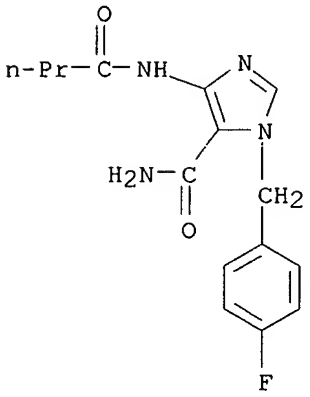
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 1-[[3,5-bis(1,1-dimethylethyl)-4-(phenylmethoxy)phenyl]methyl]-4-[(1-oxopropyl)amino]- (9CI)
MF C29 H38 N4 O3



V. Balasubramanian

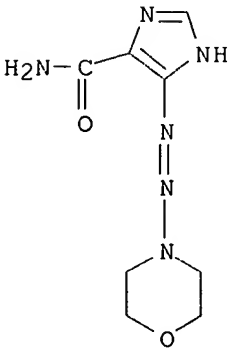
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 1-[(4-fluorophenyl)methyl]-4-[(1-oxobutyl)amino]- (9CI)
MF C15 H17 F N4 O2



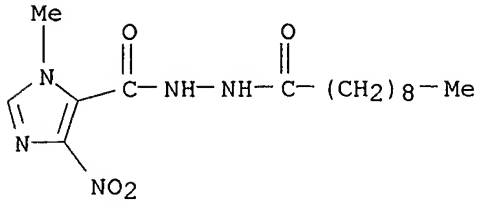
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-(4-morpholinylazo)-, monohydrochloride (9CI)
MF C8 H12 N6 O2 . Cl H



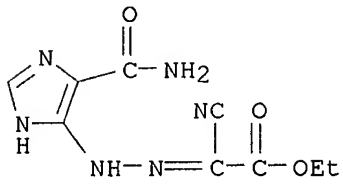
HCl

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Hydrazine, 1-decanoyl-2-[(1-methyl-4-nitroimidazol-5-yl)carbonyl]- (8CI)
MF C15 H25 N5 O4



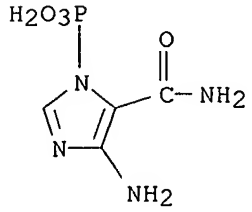
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Acetic acid, [[5-(aminocarbonyl)-1H-imidazol-4-yl]hydrazono]cyano-, ethyl ester (9CI)
MF C9 H10 N6 O3
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

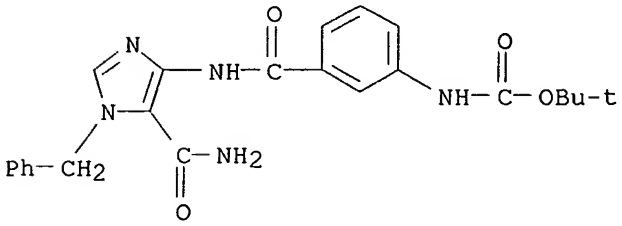
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Phosphonic acid, [4-amino-5-(aminocarbonyl)-1H-imidazol-1-yl]- (9CI)
MF C4 H7 N4 O4 P



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

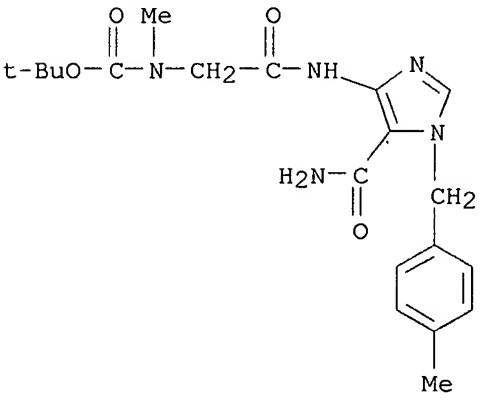
V. Balasubramanian

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Carbamic acid, [3-[[[5-(aminocarbonyl)-1-(phenylmethyl)-1H-imidazol-4-yl]amino]carbonyl]phenyl]-, 1,1-dimethylethyl ester (9CI)
MF C23 H25 N5 O4



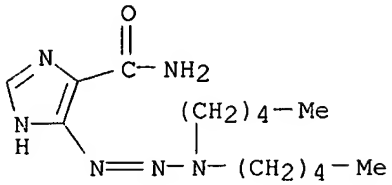
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Carbamic acid, [2-[[5-(aminocarbonyl)-1-[(4-methylphenyl)methyl]-1H-imidazol-4-yl]amino]-2-oxoethyl]methyl-, 1,1-dimethylethyl ester (9CI)
MF C20 H27 N5 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

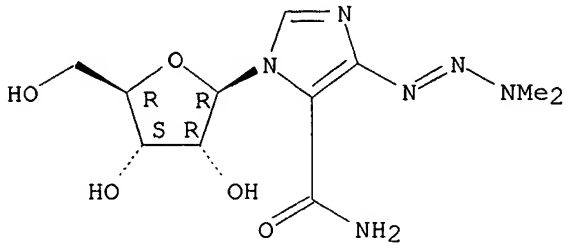
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-(3,3-dipentyl-1-triazenyl)- (9CI)
MF C14 H26 N6 O
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

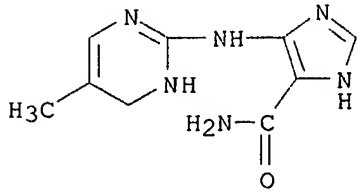
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Imidazole-5-carboxamide, 4-(3,3-dimethyl-1-triazeno)-1-.beta.-D-ribofuranosyl- (8CI)
MF C11 H18 N6 O5

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

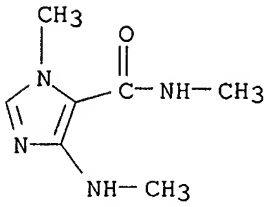
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-[(1,4-dihydro-5-methyl-2-pyrimidinyl)amino]-, monohydrochloride (9CI)
MF C9 H12 N6 O . Cl H



● HCl

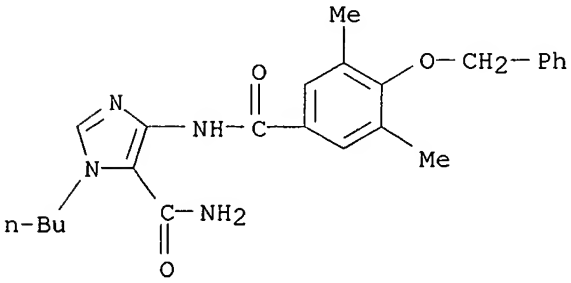
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, N,1-dimethyl-4-(methylamino)-,

monohydrochloride (9CI)
MF C7 H12 N4 O . Cl H



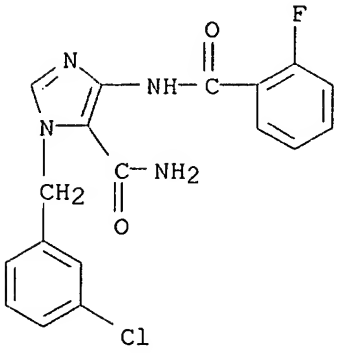
● HCl

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 1-butyl-4-[[3,5-dimethyl-4-(phenylmethoxy)benzoyl]amino]- (9CI)
MF C24 H28 N4 O3



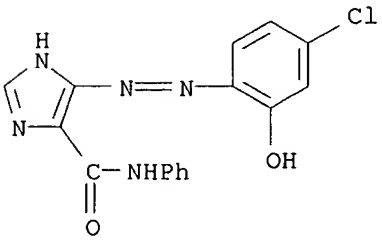
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 1-[(3-chlorophenyl)methyl]-4-[(2-fluorobenzoyl)amino]- (9CI)
MF C18 H14 Cl F N4 O2



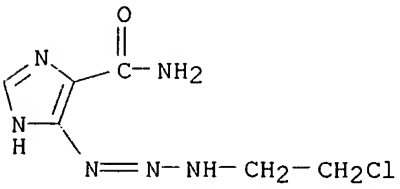
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-[(4-chloro-2-hydroxyphenyl)azo]-N-phenyl- (9CI)
MF C16 H12 Cl N5 O2



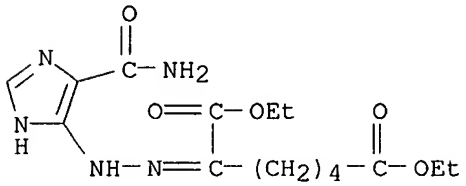
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-[3-(2-chloroethyl)-1-triazenyl]- (9CI)
MF C6 H9 Cl N6 O



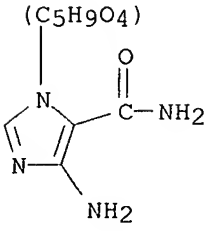
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Heptanedioic acid, 2-[[5-(aminocarbonyl)-1H-imidazol-4-yl]hydrazono]-, diethyl ester (9CI)
MF C15 H23 N5 O5

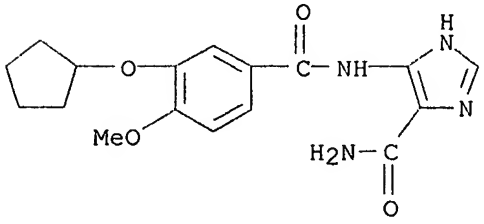


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Imidazole-5-carboxamide, 4-amino-1-ribosyl- (7CI)
MF C9 H14 N4 O5
CI IDS

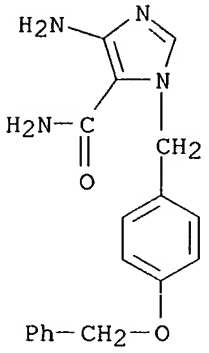


L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-4-carboxamide, 5-[[3-(cyclopentyloxy)-4-methoxybenzoyl]amino]- (9CI)
MF C17 H20 N4 O4



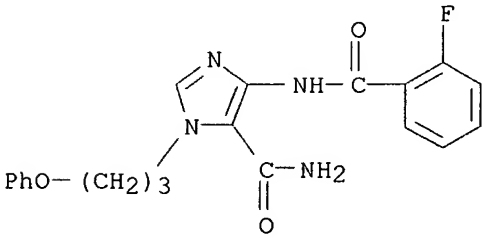
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-amino-1-[[4-(phenylmethoxy)phenyl]methyl]-
(9CI)
MF C18 H18 N4 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

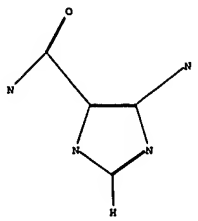
L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazole-5-carboxamide, 4-[(2-fluorobenzoyl)amino]-1-(3-phenoxypropyl)-
(9CI)
MF C20 H19 F N4 O3

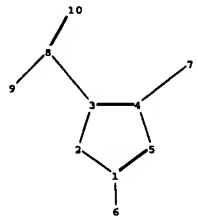


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 44 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Imidazole-5-carboxamide, N,1-dimethyl-4-(N-methylformamido)-N-nitroso-
(8CI)
MF C8 H11 N5 O3

C:\STNEXP4\QUERIES\10050488.str





chain nodes :
6 7 8 9 10
ring nodes :
1 2 3 4 5
chain bonds :
1-6 3-8 4-7 8-9 8-10
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 4-7 8-9 8-10
exact bonds :
1-6 3-8

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS